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## Strong changes in electronic transport and magnetic properties of $\text{Co}_2\text{YSi}$ Heusler alloys at $Y$ -component variation

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**Abstract.** The  $\text{Co}_2\text{YSi}$  ( $Y = \text{Ti, V, Cr, Mn, Fe, Co, Ni}$ ) Heusler alloys can manifest the properties of half-metallic ferromagnets. These compounds are promising materials for spintronics since almost 100 % spin polarization of charge carriers can be realized at room temperature. We measured the electroresistivity, magnetic and galvanomagnetic properties of the  $\text{Co}_2\text{YSi}$  ( $Y = \text{Ti, V, Cr, Mn, Fe, Co, Ni}$ ) Heusler alloys from 4.2 K to 300 K and in magnetic fields up to 100 kOe. The type, concentration and mobility of charge carriers were estimated. The  $Y$ -component variation in the  $\text{Co}_2\text{YSi}$  Heusler alloys is found to affect strongly the number of current carriers and alter the electronic band structure near the Fermi level  $E_F$  and, consequently, the electronic transport and magnetic properties of the  $\text{Co}_2\text{YSi}$  ( $Y = \text{Ti, V, Cr, Mn, Fe, Co, Ni}$ ) Heusler alloys.

### 1. Introduction

The development of modern nanoelectronics and spintronics requires the search and creation of new magnetic materials with high spin polarization of charge carriers. One of the most promising materials is half-metallic ferromagnets (HMF) [1-3]. The main feature of such materials is that in their electronic spectrum at the Fermi level there is an energy gap for one of the spin directions and its absence for another one. This can lead to 100% spin polarization of charge carriers.

Most of the Heusler alloys  $X_2YZ$  (where  $X, Y$  are 3d transition elements;  $Z$  is s-, p-elements of the Periodic Table), ordered in the  $L2_1$  crystal structure, belong to the HMF. Modern electron band structure calculations by the spin density functional method show [4-11] that in their spectrum at the Fermi level  $E_F$ , a wide ( $\sim 1$  eV) energy gap is realized in one of the subbands differing in the direction of electron spins. In recent years these alloys have been intensively investigated both by experimental methods and theoretically. A number of scientific publications is devoted to the study of optical [4], magnetic [6, 7, 8, 12, 13] and electrical [8, 14-16] properties, as well as "first-principle" calculations of the electronic band structure [4-11], which indicate that many of the Heusler HMF alloys can be used for applications.

The corresponding materials should have high Curie temperatures  $T_C$  because spintronic devices will mainly be used near the room temperature. The  $\text{Co}_2\text{YSi}$  system is appropriate materials for these purposes because in  $\text{Co}_2\text{FeSi}$  and  $\text{Co}_2\text{MnSi}$  compounds the high values of charge carriers spin polarization (about 100%) were observed near room temperature and their Curie temperatures  $T_C$  are



about 1000 K (see, for example, [17, 18]). It is quite interesting to follow the electronic and magnetic characteristics of these alloys and similar compounds of the  $\text{Co}_2\text{YSi}$  system at  $Y$ -varying. Therefore, in this work we studied the polycrystalline HMF  $\text{Co}_2\text{YSi}$  compounds, where  $Y = \text{Ti, V, Cr, Mn, Fe, Co, Ni}$ , to trend the changes in their electroresistivity, magnetic and galvanomagnetic properties.

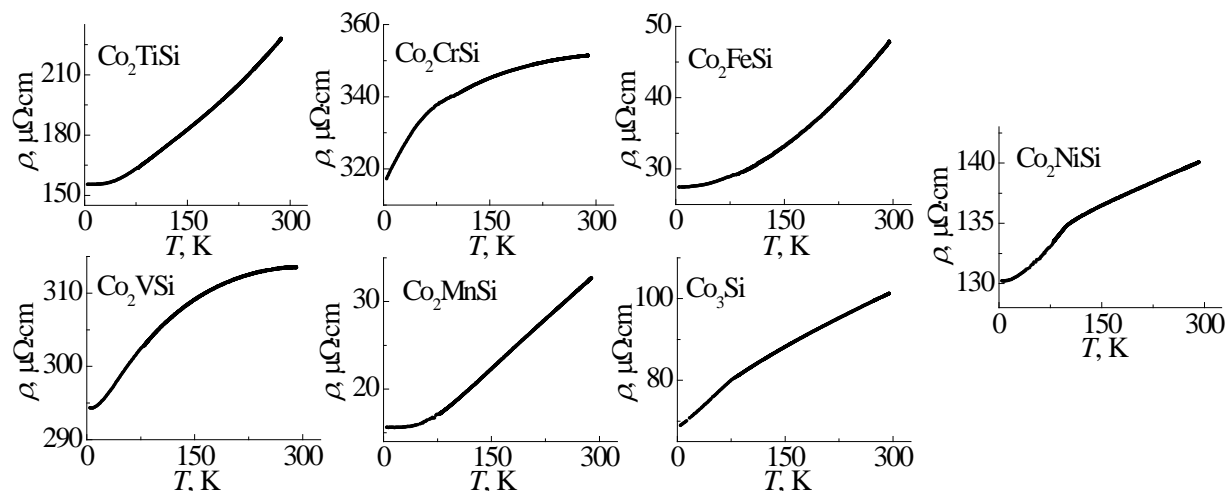
## 2. Experimental

The alloys were prepared by induced furnace. Then the result ingots of  $\text{Co}_2\text{YSi}$  ( $Y = \text{V, Cr, Fe, Co}$ ) were annealed at  $1100^\circ\text{C}$  for 3 days and quenched. The ingots of  $\text{Co}_2\text{YSi}$ , where  $Y = \text{Ti, Mn, Ni}$ , were annealed at  $800^\circ\text{C}$  for 9 days followed by cooling to room temperature. Elemental analysis was carried out by using a scanning electron microscope equipped with an EDAX X-ray microanalysis attachment. The deviation from a stoichiometric composition was revealed to be insignificant in all samples. X-ray diffraction studies showed that the samples have  $\text{L2}_1$  structure. The structural analysis was performed at the Collaborative Access Center, M.N. Mikheev Institute of Metal Physics.

The Hall Effect measurements were carried out according to a standard procedure, which is described in detail in [19, 20]. The field dependencies of the magnetization and Hall resistivity  $\rho_H(H)$  are measured at  $T = 4.2$  K in magnetic fields up to 100 kOe. The samples studied were in the form of plates with dimensions of  $\sim (0.5 \times 1.5 \times 5)$  mm. In this case, the magnetic field vector was directed strictly perpendicular to the plate plane with an accuracy of  $\pm 2$  degrees (or  $\pm 2.5\%$ ), and the electric current flowed along the largest surface of the sample. To control the asymmetry of the Hall contacts, measurements were made using a 5-point scheme [21, 22] in order to compensate for the contribution from the transverse resistivity. It was found that the data obtained using the 5- and 4-contact methods, well coincide. Therefore, further 4-pin technique was used. To determine the coefficients of the normal and anomalous Hall Effect in the same transverse geometry, we measured the field dependencies of the magnetization  $M(H)$ . The temperature dependencies of the electroresistivity were carried out at  $T = 4.2 - 300$  K with the 4-contact technique.

## 3. Results and discussion

Analysis of the temperature dependencies of the electroresistivity of samples (figure 1) showed that the alloys have different residual resistivity values  $\rho_0$  (from 20 to  $300 \mu\Omega\cdot\text{cm}$ ), and electroresistivity  $\rho(T)$  increases monotonously with temperature for all compounds. In the case of alloys with relatively low  $\rho_0$ , the electroresistivity  $\rho(T)$  changes superlinearly ( $\text{Co}_2\text{TiSi}$ ,  $\text{Co}_2\text{MnSi}$ ,  $\text{Co}_2\text{FeSi}$ ) or sublinearly ( $\text{Co}_3\text{Si}$ ,  $\text{Co}_2\text{NiSi}$ ), and for compounds with a large residual resistivity ( $\text{Co}_2\text{VSi}$ ,  $\text{Co}_2\text{CrSi}$ )  $\rho(T)$  tends to saturation at high temperatures.



**Figure 1.** Temperature dependencies of the electrical resistivity of the  $\text{Co}_2\text{YSi}$  ( $Y = \text{Ti, V, Cr, Mn, Fe, Co, Ni}$ ).

At varying the  $Y$ -component in the  $\text{Co}_2Y\text{Si}$  system ( $Y = \text{Ti, V, Cr, Mn, Fe, Co, Ni}$ ) along with the difference in residual resistivity other electronic characteristics will change, in particular, concentration of the current carriers, which should be manifested in the Hall Effect.

Since all the alloys are in the ferromagnetic state, their Hall coefficients contain both the normal  $R_0$  and the anomalous  $R_S$  components. The field dependence of Hall resistivity allows us to determine the normal and anomalous Hall coefficients by using the following equation [23]:

$$\rho_H/H = R_0 + 4\pi R_S M/H, \quad (1)$$

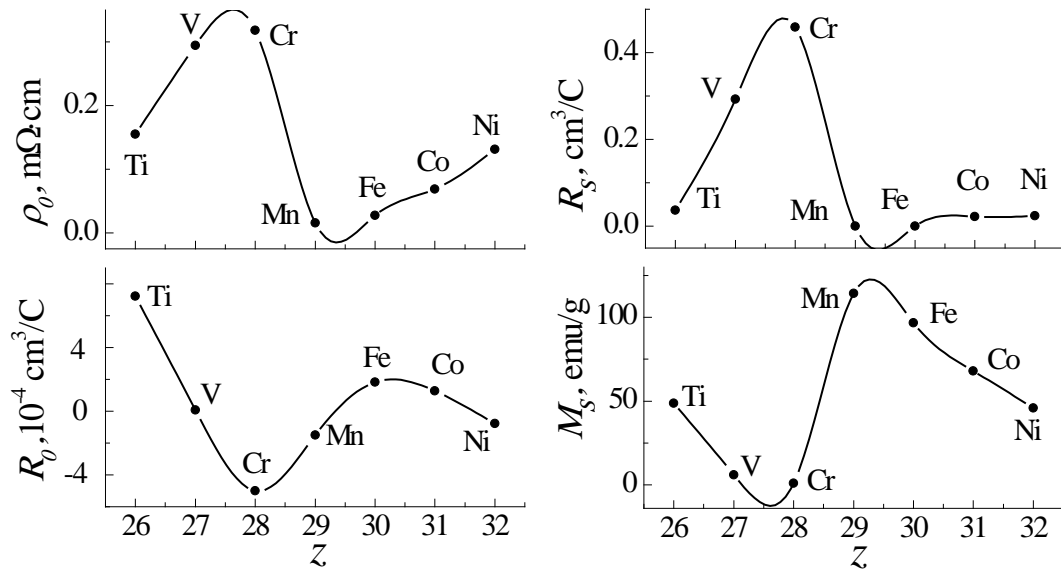
where  $\rho_H$  is the Hall resistivity,  $M$  is the magnetization. The first coefficient  $R_0$  describes the normal Hall Effect associated with the action of the Lorentz force on the movement of conduction electrons in a magnetic field  $H$ . The second coefficient  $R_S$  is associated with the presence of spin-orbit interaction and determined by the scattering processes of current carriers on the impurities and phonons and magnetic scattering centers (magnons). Table 1 shows obtained from the experimental data the type, concentration and mobility of charge carriers of  $\text{Co}_2Y\text{Si}$  samples, which are typical for metals.

**Table 1.** The electronic transport and magnetic properties of the  $\text{Co}_2Y\text{Si}$  system.

| Alloy                    | Type of charge carriers | Concentration<br>$n \cdot 10^{-22}, \text{cm}^{-3}$ | Mobility<br>$\mu, \text{cm}^2/(\text{V} \cdot \text{s})$ | $T_c, \text{K}$<br>[24, 25] |
|--------------------------|-------------------------|---|--|-----------------------------|
| $\text{Co}_2\text{TiSi}$ | holes                   | 0.9   | 4.7  | 385                         |
| $\text{Co}_2\text{VSi}$  | electrons               | 5   | 0.4  | 566                         |
| $\text{Co}_2\text{CrSi}$ | electrons               | 1   | 1.6  | 747                         |
| $\text{Co}_2\text{MnSi}$ | electrons               | 4   | 9.7  | 985                         |
| $\text{Co}_2\text{FeSi}$ | holes                   | 3   | 6.7  | 1100                        |
| $\text{Co}_3\text{Si}$   | holes                   | 5   | 1.8  | 622                         |
| $\text{Co}_2\text{NiSi}$ | electrons               | 8   | 0.6  | 589                         |

The significant changes were observed in the values of the residual electroresistivity  $\rho_0$ , the saturation magnetization  $M_S$ , the coefficients of normal  $R_0$  and anomalous  $R_S$  Hall Effects depending on the number  $z$  of valence electrons at  $Y$ -varying in the series from Ti to Ni. The observed changes in the electronic transport and magnetic properties clearly correlate with each other (figure 2).

Thus, the anomalous Hall coefficient  $R_S$  and the residual resistivity  $\rho_0$  increase near  $z = 28$ , while for the normal Hall coefficient  $R_0$  and the magnetization  $M_S$ , there is a minimum at this point. HMFs have a gap for minority spin direction and its absence for majority spin. Therefore, HMFs are considered to be sum of two parallel connected conductors (see, e.g. Refs [16, 26]). One of them with “metallic” current carriers determines by majority spin projections and another has “semiconductor” or “dielectric” state with minority spin projection. Since in the studied alloy system HMF state can arise (see, for example, [3, 17, 18, 26]), then, apparently, the presented in figure 2 correlations between  $\rho_0$ ,  $R_0$ ,  $R_S$  and  $M_S$  can be realized. In particular, it was shown in Refs [17, 18] that the  $\text{Co}_2\text{MnSi}$  and  $\text{Co}_2\text{FeSi}$  Heusler alloys are HMF compounds in which a high degree of charge carrier polarization is realized. Figure 2 shows that it is for these alloys that the maximum values of magnetization and the minimum values of residual resistivity are observed. This may be due to the fact that under these conditions the compounds predominantly contain “metallic” current carriers with spin “up”, providing a “metallic” type of conductivity and a large magnetic moment, which ultimately should lead to high spin polarization of charge carriers. It is very interesting to experimentally determine the spin polarization coefficients in these alloys, analyze their behavior when the number of valence electrons changes, and compare with the data of figure 2.

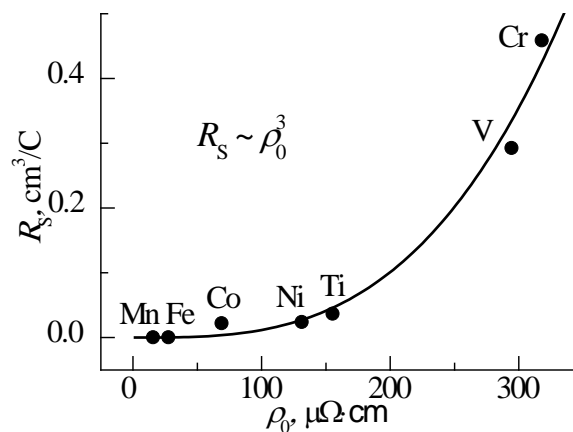


**Figure 2.** The residual electroresistivity  $\rho_0$ , the saturation magnetization  $M_s$ , the coefficients of normal  $R_0$  and anomalous  $R_s$  Hall Effect depending on the number of valence electrons  $z$  at Y-varying in the series of the  $\text{Co}_2\text{YSi}$  (Y = Ti, V, Cr, Mn, Fe, Co, Ni).

It is known [27], the anomalous Hall coefficient  $R_s$  is associated with the resistivity  $\rho$  by a power law:

$$R_s \sim \lambda_{\text{eff}} \rho^k / M_s, \quad (2)$$

where  $\lambda_{\text{eff}}$  is the constant of the spin-orbit interaction,  $k$  is an exponent depending on the scattering mechanism of charge carriers,  $M_s$  is the magnetization. The value of  $R_s$  is much higher than  $R_0$  and positive for all the samples. It is typical for ferromagnetic alloys.

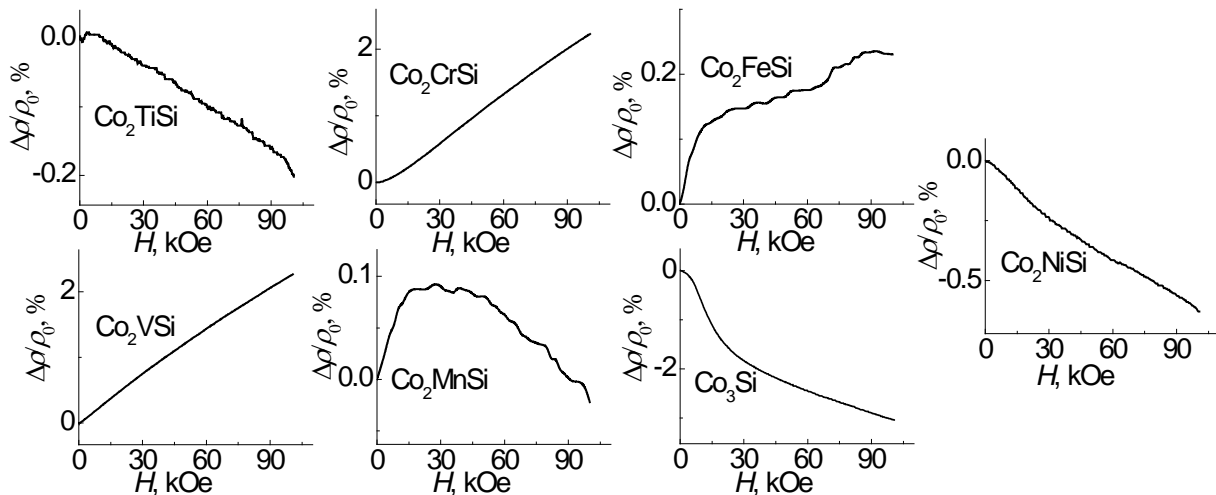


**Figure 3.** Dependence of anomalous Hall Effect vs residual resistivity.

The differences between the sign of  $R_s$  and  $R_0$  can be related to the sign of  $\lambda_{\text{eff}}$  for any scattering mechanism. At  $z$  varying, a power-law dependence of the anomalous Hall coefficient  $R_s$  on the residual electroresistivity  $\rho_0$  with the exponent  $k \approx 3$ , i.e.  $R_s \sim \rho_0^3$ , takes place (figure 3). This is inconsistent with the existing theoretical concepts, but correlates with experimental data obtained on

similar Heusler alloy systems [23]. Thus, it is necessary to take into account additional contributions to the anomalous Hall Effect. The observed correlation between the dependencies of normal Hall coefficient  $R_0$  and residual resistivity  $\rho_0$  is seemed to indicate the essential contribution in the anomalous Hall coefficient  $R_S$  of scattering processes of current carriers.

The field dependencies of the magnetoresistivity of the alloys (figure 4) have a nearly linear form (except for  $\text{Co}_2\text{MnSi}$ ) at high fields, different signs for different alloys (positive for  $\text{Co}_2\text{VSi}$ ,  $\text{Co}_2\text{CrSi}$  and  $\text{Co}_3\text{Si}$ ) and reach 2-3% (for  $\text{Co}_2\text{VSi}$ ,  $\text{Co}_2\text{CrSi}$  and  $\text{Co}_3\text{Si}$ ).



**Figure 4.** Field dependencies of the magnetoresistivity.

According to [28], two-magnon scattering processes in HMFs, along with the anomalous temperature dependencies of the ‘magnetic’ resistivity, which is due to the electron-magnon scattering, can lead to a negative linear contribution to the magnetoresistivity. Note that in the HMF  $\text{Co}_2\text{FeSi}$  alloy [26] as well as the HMF  $\text{Co}_2\text{TiSn}$  system [29] a negative contribution to the magnetoresistivity was observed. The observed field dependencies with negative part close to linear magnetoresistivity can indirectly confirm the manifestation of two-magnon scattering processes [28].

#### 4. Conclusions

The temperature dependencies of the electroresistivity, the field dependencies of the magnetoresistivity, Hall resistivity and magnetization were measured for  $\text{Co}_2\text{YSi}$  ( $Y = \text{Ti, V, Cr, Mn, Fe, Co, Ni}$ ). An analysis of the obtained results shows that the transition from  $\text{Co}_2\text{TiSi}$  to  $\text{Co}_2\text{NiSi}$ , i.e. with a variation in the number of valence electrons  $z$  within  $26 \leq z \leq 32$ , significantly changes in the sign and values of the coefficients of the normal and anomalous Hall Effect, magnetization, residual resistivity, type and concentration of current carriers and their mobilities. At the same time, the type and origin of changes in these electronic and magnetic characteristics depending on  $z$  clearly correlate with each other, and obtained values are typical for metals as well as a type of the temperature dependencies of the electrical resistivity. The electron transport properties of the alloys under consideration are largely determined not only by the scattering mechanisms of charge carriers, but in addition by the processes of electronic band structure changes near the Fermi level  $E_F$ . The studied HMF materials can be probably used for application in spintronics.

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